



wwPDB X-ray Structure Validation Summary Report ⓘ

May 12, 2020 – 11:25 pm BST

PDB ID : 2PFF
Title : Structural Insights of Yeast Fatty Acid Synthase
Authors : Xiong, Y.; Lomakin, I.B.; Steitz, T.A.
Deposited on : 2007-04-04
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

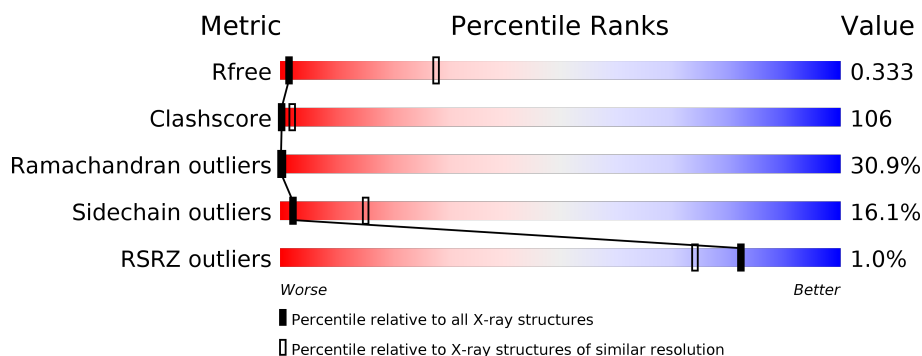
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





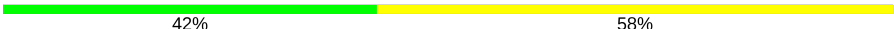
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1688	<div> <div></div> <div>27%46%22%5%</div> </div>
1	D	1688	<div> <div></div> <div>27%46%22%5%</div> </div>
1	G	1688	<div> <div></div> <div>27%46%22%5%</div> </div>
2	B	2006	<div> <div>%</div> <div>34%54%11%</div> </div>
2	E	2006	<div> <div>%</div> <div>34%54%11%</div> </div>
2	H	2006	<div> <div>%</div> <div>34%54%11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	65	 48% 52%
3	F	65	 45% 55%
3	I	65	 42% 58%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 71862 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			
1	D	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			
1	G	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2006	Total	C	N	O	S	0	0	0
			12310	7625	2253	2416	16			
2	E	2006	Total	C	N	O	S	0	0	0
			12310	7625	2253	2416	16			
2	H	2006	Total	C	N	O	S	0	0	0
			12310	7625	2253	2416	16			

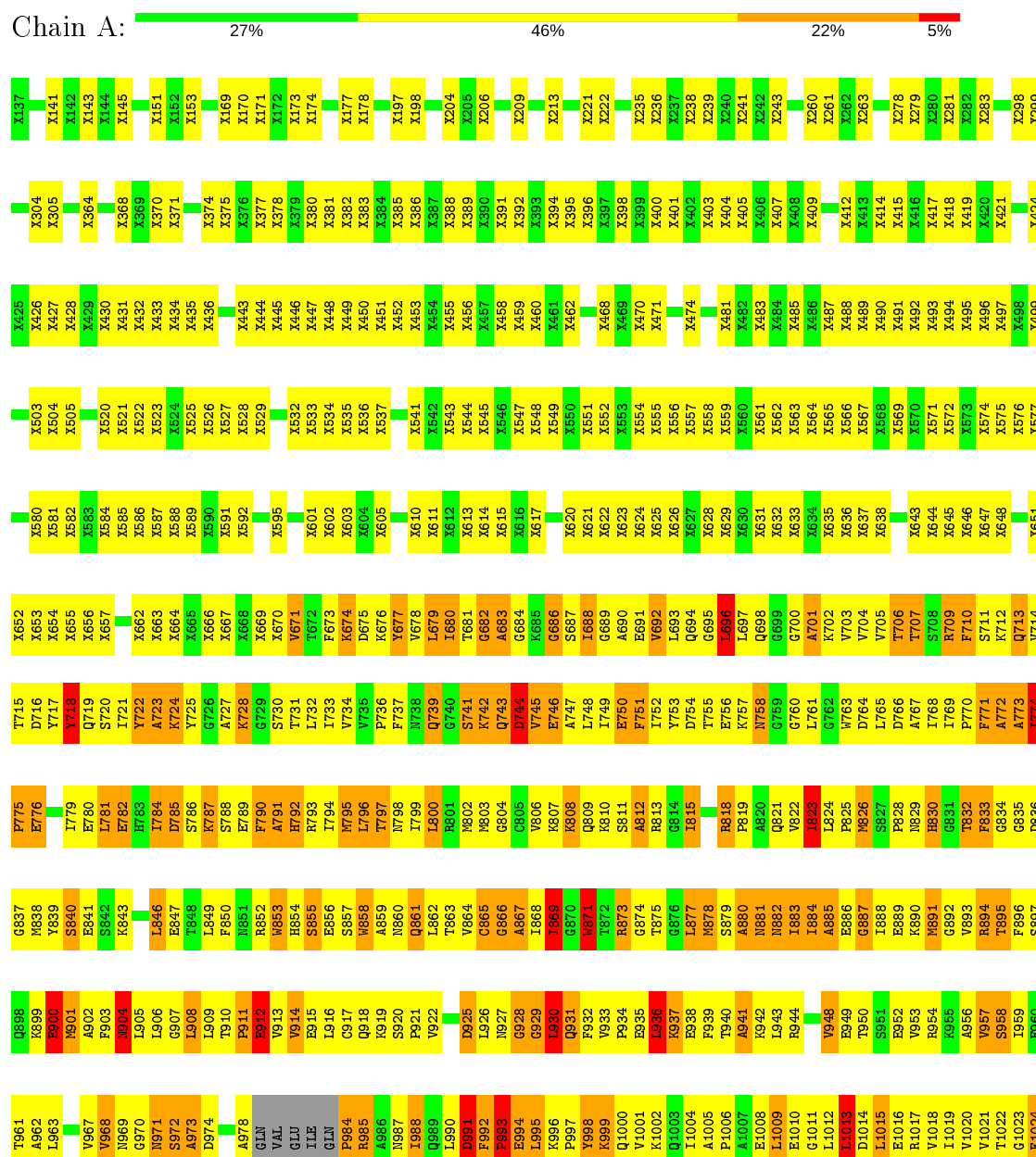
- Molecule 3 is a protein called Tail protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	65	Total	C	N	O	0	0	0
			325	195	65	65			
3	F	65	Total	C	N	O	0	0	0
			325	195	65	65			
3	I	65	Total	C	N	O	0	0	0
			325	195	65	65			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fatty acid synthase subunit alpha



- Molecule 1: Fatty acid synthase subunit alpha

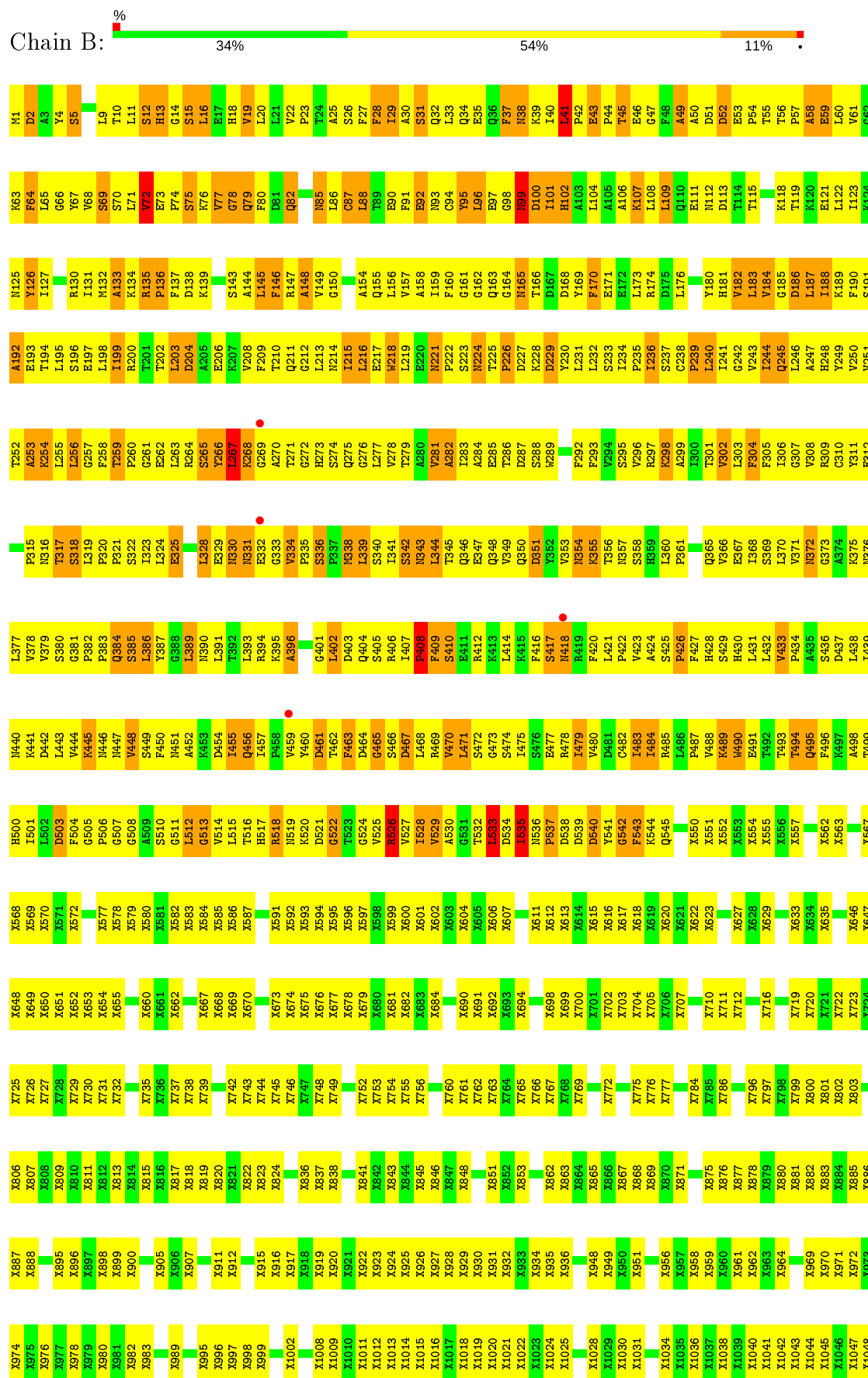
X374	X375	X376	X377	X378	X379	X380	X381	X382	X383	X384	X385	X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X397	X398	X399	X400	X401	X402	X403	X404	X405	X406	X407	X408	X409	X410	X411	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X422	X423	X424	X425	X426	X427	X428	X429	X430	X431	X432	X433	X434	X435	X436	X437	X438	X439	X440	X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500	X501	X502	X503	X504	X505	X506	X507	X508	X509	X510	X511	X512	X513	X514	X515	X516	X517	X518	X519	X520	X521	X522	X523	X524	X525	X526	X527	X528	X529	X530	X531	X532	X533	X534	X535	X536	X537	X538	X539	X540	X541	X542	X543	X544	X545	X546	X547	X548	X549	X550	X551	X552	X553	X554	X555	X556	X557	X558	X559	X560	X561	X562	X563	X564	X565	X566	X567	X568	X569	X570	X571	X572	X573	X574	X575	X576	X577	X578	X579	X580	X581	X582	X583	X584	X585	X586	X587	X588	X589	X590	X591	X592	X593	X594	X595	X596	X597	X598	X599	X600	X601	X602	X603	X604	X605	X606	X607	X608	X609	X610	X611	X612	X613	X614	X615	X616	X617	X618	X619	X620	X621	X622	X623	X624	X625	X626	X627	X628	X629	X630	X631	X632	X633	X634	X635	X636	X637	X638	X639	X640	X641	X642	X643	X644	X645	X646	X647	X648	X649	X650	X651	X652	X653	X654	X655	X656	X657	X658	X659	X660	X661	X662	X663	X664	X665	X666	X667	X668	X669	X670	X671	X672	X673	X674	X675	X676	X677	X678	X679	X680	X681	X682	X683	X684	X685	X686	X687	X688	X689	X690	X691	X692	X693	X694	X695	X696	X697	X698	X699	X700	X701	X702	X703	X704	X705	X706	X707	X708	X709	X710	X711	X712	X713	X714	X715	X716	X717	X718	X719	X720	X721	X722	X723	X724	X725	X726	X727	X728	X729	X730	X731	X732	X733	X734	X735	X736	X737	X738	X739	X740	X741	X742	X743	X744	X745	X746	X747	X748	X749	X750	X751	X752	X753	X754	X755	X756	X757	X758	X759	X760	X761	X762	X763	X764	X765	X766	X767	X768	X769	X770	X771	X772	X773	X774	X775	X776	X777	X778	X779	X780	X781	X782	X783	X784	X785	X786	X787	X788	X789	X790	X791	X792	X793	X794	X795	X796	X797	X798	X799	X800	X801	X802	X803	X804	X805	X806	X807	X808	X809	X810	X811	X812	X813	X814	X815	X816	X817	X818	X819	X820	X821	X822	X823	X824	X825	X826	X827	X828	X829	X830	X831	X832	X833	X834	X835	X836	X837	X838	X839	X840	X841	X842	X843	X844	X845	X846	X847	X848	X849	X850	X851	X852	X853	X854	X855	X856	X857	X858	X859	X860	X861	X862	X863	X864	X865	X866	X867	X868	X869	X870	X871	X872	X873	X874	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X88
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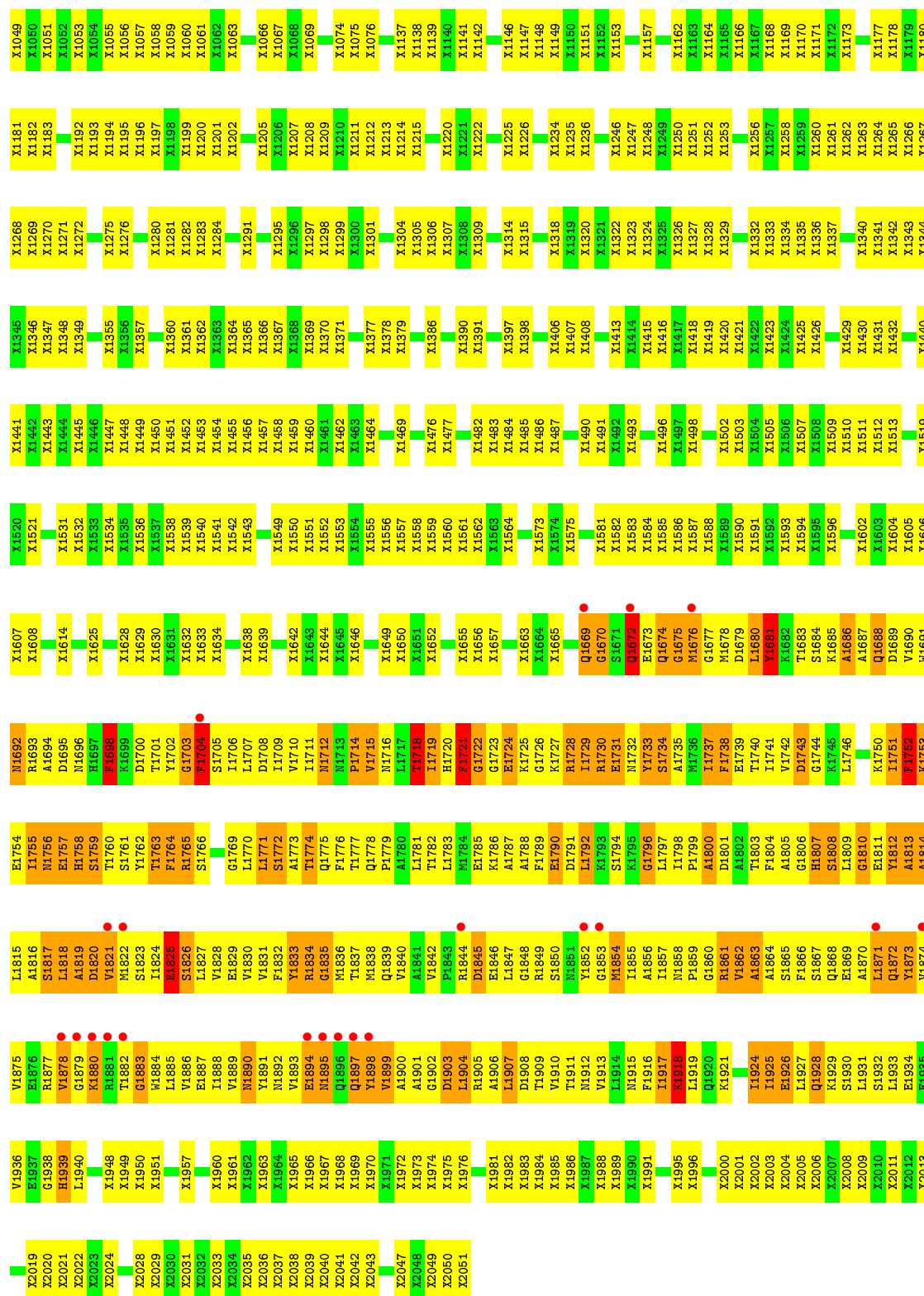


E841	E780	Q719	X655	X581	X504	X430	X368	X137	X1778	K1696	V1636	F1576	R1516	T1454
S842	L781	S720	X656	X582	X505	X431	X369	X141	X1779	L1697	R1637	Q1577	D1516	R1485
K843	E782	I721	X657	X583	X506	X432	X370	X142	X1780	F1698	V1638	F1578	P1517	R1486
S845	L844	A723	X662	X584	X520	X433	X371	X143	X1781	F1699	V1639	F1579	R1518	A1487
S846	D785	K724	X663	X585	X521	X434	X372	X144	X1782	S1700	S1640	T1581	K1519	Q1458
E847	S786	V725	X664	X586	X522	X435	X373	X145	X1783	K1701	R1641	F1580	A1520	Q1459
L848	K787	G726	X665	X587	X523	X436	X374	X146	X1784	E1702	T1642	H1582	P1521	K1460
L849	S788	A727	X666	X588	X524	X437	X375	X147	X1793	H1703	S1643	H1583	L1522	D1461
F850	E789	K728	X667	X589	X525	X438	X376	X148	X1794	A1704	F1644	P1584	G1523	V1462
N851	F790	G729	X668	X590	X526	X439	X377	X149	X1795	P1705	K1645	K1585	G1524	V1463
N852	A791	S730	X669	X591	X527	X440	X378	X150	X1796	T1706	F1646	K1586	A1525	N1465
N853	H792	T731	X670	X592	X528	X441	X379	X151	X1797	T1707	G1647	A1587	L1526	N1466
H854	R793	L732	X671	X593	X529	X442	X380	X152	X1798	D1708	Q1648	E1588	A1527	E1466
S855	I794	L733	X672	X594	X530	X443	X381	X153	X1799	E1709	K1649	G1589	T1528	L1467
E856	T795	V734	X673	X595	X531	X444	X382	X154	X1811	E1710	G1650	A1590	Y1529	E1468
S857	L796	V735	X674	X596	X532	X445	X383	X155	X1812	L1711	G1651	M1591	G1530	A1469
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N860	I799	K738	X677	X599	X535	X448	X386	X158	X1826	V1714	V1654	N1594	I1533	L1472
Q861	L800	M739	X678	X600	X536	X449	X387	X159	X1827	Y1715	V1655	G1595	D1534	E1473
L862	R801	G740	X679	X601	X537	X450	X388	X160	X1828	L1716	V1656	A1596	D1535	A1474
T863	M802	S741	X680	X602	X538	X451	X389	X161	X1853	D1717	H1657	L1597	L1536	E1475
V864	G803	K742	X681	X603	X539	X452	X390	X162	X1857	P1718	P1658	Q1598	G1537	E1476
G865	G804	Q743	X682	X604	X540	X453	X391	X163	X1860	L1719	D1659	I1599	V1538	T1477
G866	C805	D744	X683	X605	X541	X454	X392	X164	X1861	A1720	Y1660	M1601	A1539	P1478
A867	V806	V745	X684	X606	X542	X455	X393	X165	X1862	R1721	L1661	N1602	S1540	S1479
L868	K807	E746	X685	X607	X543	X456	X394	X166	X1863	Y1722	Y1662	S1602	F1541	E1480
I869	G808	A747	X686	X608	X544	X457	X395	X167	X1864	K1727	A1664	T1605	D1481	D1481
G870	Q809	L748	X687	X609	X545	X458	X396	X168	X1865	G1729	T1666	P1606	G1543	Q1482
N871	K810	I749	X688	X610	X546	X459	X397	X169	X1866	S1728	T1667	T1607	T1544	F1485
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R873	A812	F751	X690	X612	X548	X461	X399	X171	X1872	L1731	D1668	N1608	T1546	L1487
G874	G813	I752	X691	X613	X549	X462	X400	X172	X1881	T1732	Y1670	N1609	K1548	E1488
T875	G814	V753	X692	X614	X550	X463	X401	X173	X1885	F1733	A1671	N1610	N1549	T1490
G876	I815	D754	X693	X615	X551	X464	X402	X174	X1886	M1734	E1672	D1612	D1550	K1491
L877	G816	T755	X694	X616	X552	X465	X403	X175	X1887	S1735	Y1673	N1613	K1551	E1492
M878	R818	E756	X695	X617	X553	X466	X404	X176	X1888	K1736	V1674	N1614	M1552	E1493
S879	P819	K757	X696	X618	X554	X467	X405	X177	X1889	M1737	A1675	D1615	E1553	L1494
A880	A820	N758	X697	X619	X555	X468	X406	X178	X1890	Q1738	K1676	T1616	A1555	N1495
N881	Q821	G759	X698	X620	X556	X469	X407	X179	X1891	S1740	V1677	I1617	T1556	E1496
N882	V822	G760	X699	X621	X557	X470	X408	X180	X1892	D1741	S1678	L1618	I1557	A1497
I883	V823	L761	X700	X622	X558	X471	X409	X181	X1893	K1742	A1679	E1619	M1558	E1498
L884	L824	G762	X701	X623	X559	X472	X410	X182	X1894	S1743	K1680	Q1620	S1499	S1499
P825	P825	W763	X702	X624	X560	X473	X411	X183	X1895	F1621	E1622	F1621	Q1500	Q1500
E886	M826	D764	X703	X625	X561	X474	X412	X184	X1896	K1682	K1682	E1622	M1560	L1501
G887	S827	L765	X704	X626	X562	X475	X413	X185	X1897	X1745	S1683	Y1623	M1561	R1502
I888	P828	D766	X705	X627	X563	X476	X414	X186	X1898	X1746	A1684	Y1624	K1562	H1563
N889	N829	A767	X706	X628	X564	X477	X415	X187	X1899	X1747	Y1685	L1625	H1564	A1503
H890	H830	I768	X707	X629	X565	X478	X416	X188	X1900	X1748	K1686	Y1626	L1565	A1504
M891	G831	I769	X708	X630	X566	X479	X417	X189	X1901	X1750	F1687	P1627	Q1506	Q1506
G892	T832	P770	X709	X631	X567	X480	X418	X190	X1902	X1751	H1688	S1628	Q1507	Q1507
V893	F833	F771	X710	X632	X568	X481	X419	X191	X1903	X1752	F1689	S1629	G1508	W1508
G894	G834	A772	X711	X633	X569	X482	X420	X192	X1904	X1753	K1690	T1630	M1570	G1509
T895	G835	A773	X712	X634	X570	X483	X421	X193	X1905	X1754	M1691	T1631	P1571	N1510
N896	S836	I774	X713	X635	X571	X484	X422	X194	X1906	X1755	M1692	K1632	V1572	D1511
F896	D836	V775	X714	X636	X572	X485	X423	X195	X1907	X1756	L1693	T1633	I1573	F1512
S897	G837	E776	X715	X637	X573	X486	X424	X196	X1908	X1757	Y1694	D1634	G1574	Y1513
Q898	N838	E776	X716	X638	X574	X487	X425	X197	X1909	X1758	K1695	D1635	V1575	K1514
K899	G839	I777	X717	X639	X575	X488	X426	X198	X1910	X1759	M1696	P1637	G1575	
E900	S840	I779	X718	X640	X576	X489	X427	X199	X1911	X1760	F1697	S1638	V1576	
				X641	X577	X490	X428	X200	X1912	X1761	H1698	T1639	M1577	
				X642	X578	X491	X429	X201	X1913	X1762	K1699	T1640	P1578	
				X643	X579	X492	X430	X202	X1914	X1763	M1700	K1641	V1579	
				X644	X580	X493	X431	X203	X1915	X1764	L1699	T1642	G1580	
				X645	X581	X494	X432	X204	X1916	X1765	M1701	K1642	V1581	
				X646	X582	X495	X433	X205	X1917	X1766	L1699	T1643	G1581	
				X647	X583	X496	X434	X206	X1918	X1767	M1702	K1643	V1582	
				X648	X584	X497	X435	X207	X1919	X1768	L1699	T1644	G1582	
				X649	X585	X498	X436	X208	X1920	X1769	M1703	K1644	V1583	
				X650	X586	X499	X437	X209	X1921	X1770	L1699	T1645	G1583	
				X651	X587	X500	X438	X210	X1922	X1771	M1704	K1645	V1584	
				X652	X588	X501	X439	X211	X1923	X1772	L1699	T1646	G1584	
				X653	X589	X502	X440	X212	X1924	X1773	M1705	K1646	V1585	
				X654	X590	X503	X441	X213	X1925	X1774	L1699	T1647	G1585	
				X655	X591	X504	X442	X214	X1926	X1775	M1706	K1647	V1586	
				X656	X592	X505	X443	X215	X1927	X1776	L1699	T1648	G1586	
				X657	X593	X506	X444	X216	X1928	X1777	M1707	K1648	V1587	
				X658	X594	X507	X445	X217	X1929	X1778	L1699	T1649	G1587	
				X659	X595	X508	X446	X218	X1930	X1779	M1708	K1649	V1588	
				X660	X596	X509	X447	X219	X1931	X1780	L1699	T1650	G1588	
				X661	X597	X510	X448	X220	X1932	X1781	M1709	K1650	V1589	
				X662	X598	X511	X449	X221	X1933	X1782	L1699	T1651	G1589	
				X663	X599	X512	X450	X222	X1934	X1783	M1710	K1651	V1590	
				X664	X600	X513	X451	X223	X1935	X1784	L1699	T1652	G1590	
				X665	X601	X514	X452	X224	X1936	X1785	M1711	K1652	V1591	
				X666	X602	X515	X453	X225	X1937	X1786	L1699	T1653	G1591	
				X667	X603	X516	X454	X226	X1938	X1787	M1712	K1653	V1592	
				X668	X604	X517	X455	X227	X1939	X1788	L1699	T1654	G1592	
				X669	X605	X518	X456	X228	X1940	X1789	M1713	K1654	V1593	
				X670	X606	X519	X457	X229	X1941	X1790	L1699	T1655	G1593	
				X671	X607	X520	X458	X230	X1942	X1791	M1714	K1655	V1594	
				X672	X608	X521	X459	X231	X1943	X1792	L1699	T1656	G1594	
				X673	X609	X522	X460	X232	X1944	X1793	M1715	K1656	V1595	
				X674	X610	X523	X461	X233	X1945	X1794	L1699	T1657	G1595	
				X675	X611	X524	X462	X234	X1946	X1795	M1716	K1657	V1596	
				X676	X612	X525	X463	X235	X1947	X1796	L1699	T1658	G1596	
				X677	X613	X526	X464	X236	X1948	X1797	M1717	K1658	V1597	
				X678	X614	X527	X465	X237	X1949	X1798	L1699	T1659	G1597	
				X679	X615	X528	X466	X238	X1950	X1799	M1718	K		

X1773	I1693	T1633	I1573	F1512	Q1451	A1390	G1330	V1270	P1210	D1150	D1088	P1029	X1773	X1773
X1778	Y1694	D1634	G1574	Y1513	L1452	D1391	G1331	Q1271	I1211	K1151	V1089	P1028	X1778	X1778
X1779	M1695	G1635	F1575	R1514	T1453	L1392	Y1332	M1272	T1212	Y1152	K1090	W1030	X1779	X1779
X1780	K1696	V1636	F1576	R1515	T1454	A1393	D1333	D1273	T1213	D1153	A1091	G1031	X1780	X1780
X1781	L1697	R1637	Q1577	P1516	R1455	L1394	D1334	I1274	F1214	F1154	Y1092	S1032	X1781	X1781
X1782	L1698	K1638	K1578	P1517	R1456	K1395	F1335	L1275	V1215	F1155	Y1093	A1033	X1782	X1782
X1783	L1699	V1639	F1579	R1518	Q1457	M1396	Q1336	Q1276	L1216	E1156	E1094	R1034	X1783	X1783
X1784	S1700	S1640	L1580	T1519	Q1458	G1397	E1337	D1277	V1217	L1157	T1095	T1036	X1784	X1784
X1793	K1701	T1641	T1581	A1520	I1459	V1398	E1338	S1278	S1218	P1158	S1096	R1036	X1793	X1793
X1794	E1702	T1642	G1582	P1521	K1460	P1399	F1339	F1279	V1219	E1159	L1097	W1037	X1794	X1794
X1795	A1704	S1643	H1583	L1522	D1461	I1400	S1340	I1280	T1220	T1160	L1098	E1038	X1795	X1795
X1799	P1705	F1644	P1584	G1524	V1462	Y1401	F1341	H1281	E1221	G1161	E1099	M1039	X1799	X1799
X1811	E1710	G1645	K1585	G1524	E1464	G1402	E1342	T1282	A1222	E1162	H1100	E1040	X1811	X1811
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X1813	E1712	G1647	A1587	L1526	N1465	V1404	G1344	S1284	I1224	S1164	G1102	F1042	X1813	X1813
X1826	D1713	K1648	A1588	A1527	N1466	A1405	N1345	E1285	I1225	Y1165	I1103	G1043	X1826	X1826
X1827	Y1714	K1649	G1589	Y1528	L1467	M1406	M1346	M1286	G1226	K1166	L1104	E1044	X1827	X1827
X1853	Y1715	V1655	G1595	F1529	E1468	A1407	K1347	V1287	G1227	L1167	L1105	F1045	X1853	X1853
X1857	L1716	L1656	A1596	D1535	E1474	K1413	L1353	S1293	M1234	Y1174	N1112	E1052	X1857	X1857
X1866	D1717	L1657	L1597	L1536	E1475	I1414	E1354	S1294	M1234	Y1174	N1112	E1052	X1866	X1866
X1872	P1718	P1658	Q1598	G1537	E1476	I1414	E1355	S1295	Y1235	T1175	G1113	M1053	X1872	X1872
X1881	E1719	D1659	L1599	V1538	I1477	S1417	F1356	G1296	K1236	P1176	E1114	A1054	X1881	X1881
X1885	A1720	L1660	A1539	F1537	Y1418	V1418	F1357	P1297	Y1237	K1177	N1115	W1055	X1885	X1885
X1886	Y1721	L1661	N1601	S1540	S1479	P1419	H1388	I1298	V1238	L1178	K1116	I1056	X1886	X1886
X1887	E1722	Y1662	S1602	F1541	E1480	A1420	T1382	I1292	Y1232	T1172	L1110	C1050	X1887	X1887
X1887	Y1722	G1663	G1603	H1542	D1481	P1421	R1360	K1299	H1239	L1179	E1117	M1057	X1887	X1887
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X1887	S1728	L1665	F1605	T1544	Q1482	K1423	P1362	V1302	E1242	D1182	E1120	I1060	X1887	X1887
X1887	G1729	T1666	F1607	S1545	L1486	G1424	A1364	G1303	V1243	R1183	M1121	S1061	X1887	X1887
X1887	S1730	E1667	T1546	F1546	L1486	T1425	A1304	A1304	G1244	L1184	I1122	Y1062	X1887	X1887
X1887	L1731	D1668	N1608	K1547	L1487	L1426	M1365	C1305	M1245	V1185	I1126	H1064	X1887	X1887
X1887	T1732	R1669	R1609	A1548	E1488	T1427	S1366	A1306	G1246	A1186	V1127	G1065	X1887	X1887
X1887	E1733	Y1670	N1610	M1549	E1489	T1428	R1367	T1307	S1247	G1187	V1127	G1065	X1887	X1887
X1887	N1734	L1671	D1612	K1551	T1490	A1429	P1368	S1308	G1248	Q1188	E1128	R1066	X1887	X1887
X1887	S1735	E1572	N1613	M1552	E1492	R1430	A1369	V1309	S1249	I1189	E1129	L1067	X1887	X1887
X1887	K1736	Y1673	N1614	E1553	I1493	H1432	T1370	E1310	M1251	P1190	D1130	K1068	X1887	X1887
X1887	N1737	V1674	V1614	E1553	I1493	H1432	T1371	S1311	M1251	T1191	L1131	G1069	X1887	X1887
X1887	Q1738	A1675	D1615	S1554	H1494	H1433	T1372	V1312	G1252	G1192	E1132	R1070	X1887	X1887
X1887	S1739	K1676	K1616	A1555	N1495	S1434	R1373	D1313	G1253	M1193	P1133	P1071	X1887	X1887
X1887	S1740	V1677	L1617	T1556	E1496	S1435	H1374	I1314	V1254	N1194	F1134	Y1072	X1887	X1887
X1887	D1742	S1678	L1618	I1557	E1497	V1436	G1375	G1315	S1255	A1195	E1135	T1073	X1887	X1887
X1887	R1743	A1679	E1619	N1558	E1498	K1437	F1376	V1316	A1256	K1196	A1136	G1074	X1887	X1887
X1887	Y1744	R1680	Q1620	E1559	S1499	Y1438	M1377	E1317	L1257	T1197	S1137	W1075	X1887	X1887
X1887	X1745	E1681	F1621	M1560	Q1500	A1439	E1378	T1318	R1258	Y1198	K1138	D1077	X1887	X1887
X1887	X1745	K1682	E1622	M1561	L1501	S1440	A1379	I1319	G1259	G1199	E1139	R1077	X1887	X1887
X1887	X1746	S1683	Y1623	K1562	R1502	P1441	Q1380	L1320	M1260	I1200	T1140	S1078	X1887	X1887
X1887	X1747	A1684	V1624	H1563	A1503	M1442	S1321	S1321	F1261	S1201	A1141	K1079	X1887	X1887
X1887	X1748	Y1685	L1625	L1564	A1504	L1443	A1382	G1322	R1262	D1202	E1142	T1080	X1887	X1887
X1887	X1749	K1686	Y1626	G1565	Q1505	N1444	G1383	K1323	D1263	D1203	Q1143	K1081	X1887	X1887
X1887	X1750	P1687	P1628	R1566	Q1507	M1445	I1394	A1324	R1264	I1204	F1144	E1082	X1887	X1887
X1887	X1750	F1688	S1628	Q1507	Q1507	K1446	Q1385	R1325	R1265	I1205	K1145	P1083	X1887	X1887
X1887	X1754	H1689	K1629	G1508	W1508	Y1447	I1386	I1326	R1266	S1206	H1146	V1084	X1887	X1887
X1887	X1761	N1690	T1630	N1570	G1509	R1448	I1387	G1327	D1267	Q1207	A1025	D1085	X1887	X1887
X1887	X1762	M1692	K1632	V1572	D1511	R1450	Q1389	V1329	P1269	D1209	G1149	K1087	X1887	X1887

• Molecule 2: Fatty acid synthase subunit beta





• Molecule 2: Fatty acid synthase subunit beta



X973	X974	X975	X976	X977	X978	X982	X983	X989	X997	X998	X995	X996	X997	X998	X999	X1002	X1008	X1009	X1010	X1011	X1012	X1013	X1014	X1015	X1016	X1017	X1018	X1019	X1020	X1021	X1022	X1023	X1024	X1025	X1028	X1029	X1030	X1031	X1034	X1035	X1036	X1037	X1038	X1039	X1040	X1041	X1042	X1043	X1044	X1045	X1046	X1047	X1048	X1049	X1050																																																																																																																																																																																																																																																																																																																																																																																																																																													
X897	X898	X899	X900	X905	X906	X907	X817	X818	X819	X820	X821	X822	X823	X824	X825	X836	X841	X842	X843	X844	X845	X846	X847	X848	X851	X852	X853	X862	X863	X864	X865	X866	X867	X868	X869	X870	X871	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X887	X888	X895	X896	X897	X898	X899	X900	X901	X902	X903	X904	X905	X906	X907	X908	X909	X910	X911	X912	X913	X914	X915	X916	X917	X918	X919	X920	X921	X922	X923	X924	X925	X926	X927	X928	X929	X930	X931	X932	X933	X934	X935	X936	X939	X946	X947	X948	X949	X950	X951	X956	X957	X958	X959	X960	X961	X962	X963	X964	X965	X966	X969	X970	X971	X972																																																																																																																																																																																																																																																																																																																																																																																			
X809	X810	X811	X812	X813	X814	X815	X816	X817	X818	X819	X820	X821	X822	X823	X824	X825	X836	X841	X842	X843	X844	X845	X846	X847	X848	X851	X852	X853	X862	X863	X864	X865	X866	X867	X868	X869	X870	X871	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X887	X888	X895	X896	X897	X898	X899	X900	X901	X902	X903	X904	X905	X906	X907	X908	X909	X910	X911	X912	X913	X914	X915	X916	X917	X918	X919	X920	X921	X922	X923	X924	X925	X926	X927	X928	X929	X930	X931	X932	X933	X934	X935	X936	X939	X946	X947	X948	X949	X950	X951	X956	X957	X958	X959	X960	X961	X962	X963	X964	X965	X966	X969	X970	X971	X972																																																																																																																																																																																																																																																																																																																																																																																		
X726	X727	X728	X729	X730	X731	X732	X735	X736	X737	X738	X739	X742	X743	X744	X745	X746	X747	X748	X749	X752	X753	X754	X755	X756	X760	X761	X762	X763	X764	X765	X766	X767	X768	X769	X770	X771	X772	X775	X776	X777	X784	X785	X786	X787	X788	X789	X790	X791	X792	X793	X794	X795	X796	X797	X798	X799	X800	X801	X802	X803	X806	X807	X808	X809	X810	X811	X812	X813	X814	X815	X816	X817	X818	X819	X820	X821	X822	X823	X824	X825	X826	X827	X828	X829	X830	X831	X832	X833	X834	X835	X836	X837	X838	X839	X840	X841	X842	X843	X844	X845	X846	X847	X848	X849	X850	X851	X852	X853	X854	X855	X856	X857	X858	X859	X860	X861	X862	X863	X864	X865	X866	X867	X868	X869	X870	X871	X872	X873	X874	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X885	X886	X887	X888	X889	X890	X891	X892	X893	X894	X895	X896	X897	X898	X899	X900	X901	X902	X903	X904	X905	X906	X907	X908	X909	X910	X911	X912	X913	X914	X915	X916	X917	X918	X919	X920	X921	X922	X923	X924	X925	X926	X927	X928	X929	X930	X931	X932	X933	X934	X935	X936	X939	X946	X947	X948	X949	X950	X951	X956	X957	X958	X959	X960	X961	X962	X963	X964	X965	X966	X969	X970	X971	X972																																																																																																																																																																																																																																																																															
X650	X651	X652	X653	X654	X655	X656	X657	X660	X661	X662	X667	X668	X669	X670	X674	X675	X676	X677	X678	X679	X680	X681	X682	X683	X684	X685	X686	X689	X691	X692	X693	X694	X698	X699	X700	X701	X702	X703	X704	X705	X706	X707	X711	X712	X716	X719	X720	X721	X722	X723	X724	X725	X726	X727	X728	X729	X730	X731	X732	X735	X736	X737	X738	X739	X742	X743	X744	X745	X746	X747	X748	X749	X752	X753	X754	X755	X756	X760	X761	X762	X763	X764	X765	X766	X767	X768	X769	X770	X771	X772	X775	X776	X777	X784	X785	X786	X787	X788	X789	X790	X791	X792	X793	X794	X795	X796	X797	X798	X799	X800	X801	X802	X803	X806	X807	X808	X809	X810	X811	X812	X813	X814	X815	X816	X817	X818	X819	X820	X821	X822	X823	X824	X825	X826	X827	X828	X829	X830	X831	X832	X833	X834	X835	X836	X837	X838	X839	X840	X841	X842	X843	X844	X845	X846	X847	X848	X849	X850	X851	X852	X853	X854	X855	X856	X857	X858	X859	X860	X861	X862	X863	X864	X865	X866	X867	X868	X869	X870	X871	X872	X873	X874	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X885	X886	X887	X888	X889	X890	X891	X892	X893	X894	X895	X896	X897	X898	X899	X900	X901	X902	X903	X904	X905	X906	X907	X908	X909	X910	X911	X912	X913	X914	X915	X916	X917	X918	X919	X920	X921	X922	X923	X924	X925	X926	X927	X928	X929	X930	X931	X932	X933	X934	X935	X936	X939	X946	X947	X948	X949	X950	X951	X956	X957	X958	X959	X960	X961	X962	X963	X964	X965	X966	X969	X970	X971	X972																																																																																																																																																																																																																										
X501	X502	D503	F504	G505	P506	G507	A508	S509	S510	G511	L512	G513	V514	L515	T516	R517	R518	N519	K520	D521	G522	T523	G524	V525	R526	V527	L528	S529	D530	L531	R532	L533	R534	D535	L536	R537	L538	R539	D540	L541	R542	L543	R544	G545	L546	R547	L548	R549	D550	L551	R552	L553	R554	G555	L556	R557	L558	R559	D560	L561	R562	L563	R564	G565	L566	R567	L568	R569	D570	L571	R572	L573	R574	G575	L576	R577	L578	R579	D580	L581	R582	L583	R584	G585	L586	R587	L588	R589	D590	L591	R592	L593	R594	G595	L596	R597	L598	R599	D600	L601	R602	L603	R604	G605	L606	R607	L608	R609	D610	L611	R612	L613	R614	G615	L616	R617	L618	R619	D620	L621	R622	L623	R624	G625	L626	R627	L628	R629	D630	L631	R632	L633	R634	G635	L636	R637	L638	R639	D640	L641	R642	L643	R644	G645	L646	R647	L648	R649	D650	L651	R652	L653	R654	G655	L656	R657	L658	R659	D660	L661	R662	L663	R664	G665	L666	R667	L668	R669	D670	L671	R672	L673	R674	G675	L676	R677	L678	R679	D680	L681	R682	L683	R684	G685	L686	R687	L688	R689	D690	L691	R692	L693	R694	G695	L696	R697	L698	R699	D699	L700	R701	L702	R703	L704	R705	L706	R707	L711	R712	L716	R719	L720	R721	L722	R723	L724	R725	X650	X651	X652	X653	X654	X655	X656	X657	X660	X661	X662	X667	X668	X669	X670	X674	X675	X676	X677	X678	X679	X680	X681	X682	X683	X684	X685	X686	X689	X691	X692	X693	X694	X698	X699	X700	X701	X702	X703	X704	X705	X706	X707	X711	X712	X716	X719	X720	X721	X722	X723	X724	X725	X726	X727	X728	X729	X730	X731	X732	X735	X736	X737	X738	X739	X742	X743	X744	X745	X746	X747	X748	X749	X752	X753	X754	X755	X756	X760	X761	X762	X763	X764	X765	X766	X767	X768	X769	X770	X771	X772	X775	X776	X777	X784	X785	X786	X787	X788	X789	X790	X791	X792	X793	X794	X795	X796	X797	X798	X799	X800	X801	X802	X803	X806	X807	X808	X809	X810	X811	X812	X813	X814	X815	X816	X817	X818	X819	X820	X821	X822	X823	X824	X825	X826	X827	X828	X829	X830	X831	X832	X833	X834	X835	X836	X837	X838	X839	X840	X841	X842	X843	X844	X845	X846	X847	X848	X849	X850	X851	X852	X853	X854	X855	X856	X857	X858	X859	X860	X861	X862	X863	X864	X865	X866	X867	X868	X869	X870	X871	X872	X873	X874	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X885	X886	X887	X888	X889	X890	X891	X892	X893	X894	X895	X896	X897	X898	X899	X900	X901	X902	X903	X904	X905	X906	X907	X908	X909	X910	X911	X912	X913	X914	X915	X916	X917	X918	X919	X920	X921	X922	X923	X924	X925	X926	X927	X928	X929	X930	X931	X932	X933	X934	X935	X936	X939	X946	X947	X948	X949	X950	X951	X956	X957	X958	X959	X960	X961	X962	X963	X964	X965	X966	X969	X970	X971	X972
K441	D442	L443	V444	K445	L446	D447	V448	S449	F450	L451	A452	K453	D454	L455	T456	R457	R458	N459	K460	D461	G462	T463	G464	V465	R466	V467	L468	R469	D470	L471	S472	K473	L474	R475	S476	E477	R478	L479	D480	L481	P482	C483	I484	R485	L486	P487	V488	K489	L490	E491	T492	T493	T494	P495	P496	K497	A498	T499	H500	K441	D442	L443	V444	K445	L446	D447	V448	S449	F450	L451	A452	K453	D454	L455	T456	R457	R458	N459	K460	D461	G462	T463	G464	V465	R466	V467	L468	R469	D470	L471	S472	K473	L474	R475	S476	E477	R478	L479	D480	L481	P482	C483	I484	R485	L486	P487	V488	K489	L490	E491	T492	T493	T494	P495	P496	K497	A498	T499	H500																																																																																																																																																																																																																																																																																																																																																																													
L377	V378	S379	G380	L381	P382	P383	Q384	S385	L386	Y387	G388	L389	N390	E391	T392	R393	R394	K395	A396	G401	L402	D403	Q404	S405	R406	L407	P408	F409	S410	E411	R412	K415	F416	S417	R418	L419	D420	L421	P422	V423	A424	S425	P426	F427	H428	S429	H430	L431	L432	V433	P434	A435	G436	D437	L438	I439	N440	L377	V378	S379	G380	L381	P382	P383	Q384	S385	L386	Y387	G388	L389	N390	E391	T392	R393	R394	K395	A396	G401	L402	D403	Q404	S405	R406	L407	P408	F409	S410	E411	R412	K415	F416	S417	R418	L419	D420	L421	P422	V423	A424	S425	P426	F427	H428	S429	H430	L431	L432	V433	P434	A435	G436	D437	L438	I439	N440																																																																																																																																																																																																																																																																																																																																																																																	
V251	T252	K253	K254	L255	L256	G257	F258	T259	G260	P261	E262	L263	R264	S265	Y266	K267	K268	G269	A270	G271	G272	H273	T274	Q275	G276	V277	L278	T279	V281	P282	A282	L283	E284	E285</																																																																																																																																																																																																																																																																																																																																																																																																																																																																		

X1051	X1052	X1053	X1054	X1055	X1056	X1057	X1058	X1059	X1060	X1061	X1062	X1063	X1066	X1067	X1068	X1069	X1074	X1075	X1076	X1077	X1078	X1079
X1180	X1181	X1182	X1183	X1192	X1193	X1194	X1195	X1196	X1197	X1198	X1199	X1200	X1201	X1202	X1205	X1206	X1207	X1208	X1209	X1210	X1211	X1212
X1265	X1266	X1267	X1268	X1269	X1270	X1271	X1272	X1275	X1276	X1280	X1281	X1282	X1283	X1284	X1291	X1295	X1296	X1297	X1298	X1299	X1300	X1301
X1344	X1345	X1346	X1347	X1348	X1349	X1355	X1356	X1357	X1360	X1361	X1362	X1369	X1370	X1371	X1377	X1378	X1379	X1386	X1389	X1390	X1391	X1393
X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1462	X1463	X1464	X1469	X1476	X1477	X1482	X1483
X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1558
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X1589	X1590	X1591	X1592	X1593	X1594	X1595	X1596	X1602	X1603	X1604	X1605	X1606	X1607	X1608	X1669	X1670	X1671	X1672	X1673	X1674	X1675	X1676
X1677	X1678	X1679	X1680	X1681	X1682	X1683	X1684	X1685	X1686	X1687	X1688	X1689	X1690	X1691	X1692	X1693	X1694	X1695	X1696	X1697	X1698	X1699
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X1792	X1793	X1794	X1795	X1796	X1797	X1798	X1799	X1800	X1801	X1802	X1803	X1804	X1805	X1806	X1807	X1808	X1809	X1810	X1811	X1812	X1813	X1814
X1815	X1816	X1817	X1818	X1819	X1820	X1821	X1822	X1823	X1824	X1825	X1826	X1827	X1828	X1829	X1830	X1831	X1832	X1833	X1834	X1835	X1836	X1837
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X1861	X1862	X1863	X1864	X1865	X1866	X1867	X1868	X1869	X1870	X1871	X1872	X1873	X1874	X1875	X1876	X1877	X1878	X1879	X1880	X1881	X1882	X1883
X1884	X1885	X1886	X1887	X1888	X1889	X1890	X1891	X1892	X1893	X1894	X1895	X1896	X1897	X1898	X1899	X1900	X1901	X1902	X1903	X1904	X1905	X1906
X1907	X1908	X1909	X1910	X1911	X1912	X1913	X1914	X1915	X1916	X1917	X1918	X1919	X1920	X1921	X1922	X1923	X1924	X1925	X1926	X1927	X1928	X1929
X1930	X1931	X1932	X1933	X1934	X1935	X1936	X1937	X1938	X1939	X1940	X1941	X1942	X1943	X1944	X1945	X1946	X1947	X1948	X1949	X1950	X1951	X1952
X1953	X1954	X1955	X1956	X1957	X1958	X1959	X1960	X1961	X1962	X1963	X1964	X1965	X1966	X1967	X1968	X1969	X1970	X1971	X1972	X1973	X1974	X1975
X1976	X1977	X1978	X1979	X1980	X1981	X1982	X1983	X1984	X1985	X1986	X1987	X1988	X1989	X1990	X1991	X1992	X1993	X1994	X1995	X1996	X1997	X1998
X1999	X2000	X2001	X2002	X2003	X2004	X2005	X2006	X2007	X2008	X2009	X2010	X2011	X2012	X2013	X2014	X2015	X2016	X2017	X2018	X2019	X2020	X2021
X2022	X2023	X2024	X2025	X2026	X2027	X2028	X2029	X2030	X2031	X2032	X2033	X2034	X2035	X2036	X2037	X2038	X2039	X2040	X2041	X2042	X2043	X2044
X2045	X2046	X2047	X2048	X2049	X2050	X2051	X2052	X2053	X2054	X2055	X2056	X2057	X2058	X2059	X2060	X2061	X2062	X2063	X2064	X2065	X2066	X2067

• Molecule 2: Fatty acid synthase subunit beta

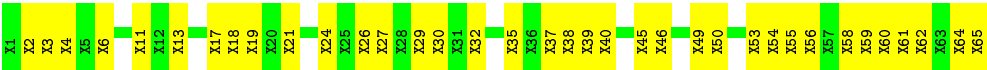




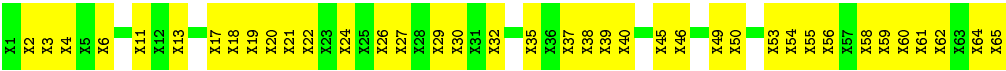
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X2012	X1053	X1182	X1270	X1347	X1441	X1521	X1605	V1890	F1752	A1813	V1873	E1934	X2021
X2013	X1054	X1183	X1271	X1348	X1442	X1522	X1606	W1691	X1753	A1814	V1874	E1935	X2022
	X1055		X1272	X1349	X1443	X1523	X1607	M1692	E1754	L1815	E1875	V1936	
X2019	X1056	X1192	X1275	X1355	X1444	X1524	X1608	R1693	I1755	A1816	E1876	G1938	X2023
X2020	X1057	X1193	X1276	X1356	X1445	X1525	X1614	A1894	M1756	S1817	R1877	G1939	X2024
X2021	X1058	X1194	X1277	X1357	X1446	X1526		D1895	E1757	L1818	V1878	H1939	
X2022	X1059	X1195		X1358	X1447	X1527	X1615	M1696	H1758	A1819	E1879	L1940	
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	X1062	X1198	X1282	X1362	X1450	X1530	X1630	D1700	S1761	M1822	G1883	X1949	
X2028	X1063	X1199	X1283	X1363	X1451	X1531	X1631	T1701	Y1762	S1823	W1884	X1950	
X2029		X1200	X1284	X1364	X1452	X1532	X1632	F1763	F1764	E1824		X1951	
X2030	X1066	X1201		X1365	X1453	X1533	X1633	G1703	R1765	S1825			
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X2033	X1069	X1206	X1295	X1368	X1456	X1536	X1638	I1706	G1769	V1828	L1888	X1960	
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	X1139	X1217	X1308	X1387	X1467	X1547	X1649	V1717	A1780	V1840	A1900	X1971	
X2047	X1140	X1218	X1309	X1388	X1476	X1548	X1650	L1718	L1781	A1841	A1901	X1972	
X2048	X1141	X1219	X1310	X1389	X1477	X1549	X1651	R1719	T1782	V1842	G1902	X1973	
X2049	X1142	X1220	X1311	X1390	X1478	X1550	X1652	H1720	L1783	F1843	D1903	X1974	
X2050	X1146	X1225	X1312	X1391	X1482	X1551	X1653	I1721	M1784	L1844	R1904	X1975	
X2051	X1147	X1226	X1313	X1392	X1483	X1552	X1654	G1722	E1785	D1845	A1905	X1976	
	X1148	X1234	X1314	X1393	X1484	X1553	X1655	E1723	K1786	E1846	A1906		
	X1149	X1235	X1315	X1394	X1485	X1554	X1656	G1724	A1787	L1847	I1907	X1981	
X1150	X1236	X1249	X1316	X1395	X1486	X1555	X1657	K1725	A1788	G1848	D1908	X1982	
X1151	X1246	X1250	X1317	X1396	X1487	X1556	X1658	G1726	F1789	A1849	T1909	X1983	
X1152	X1247	X1251	X1318	X1397	X1488	X1557	X1659	K1727	E1790	S1850	V1910	X1984	
X1153	X1248	X1252	X1319	X1398	X1489	X1558	X1660	D1728	D1791	M1851	T1911	X1985	
	X1253	X1263	X1320	X1399	X1490	X1559	X1661	R1729	L1792	Y1852	N1912	X1986	
	X1256	X1264	X1321	X1400	X1491	X1560	X1662	R1730	G1793	G1853	V1913	X1987	
	X1257	X1265	X1322	X1401	X1492	X1561	X1663	E1731	S1794	M1854	L1914	X1988	
	X1258	X1266	X1323	X1402	X1493	X1562	X1664	E1732	K1795	L1855	V1915	X1989	
	X1259	X1267	X1324	X1403	X1494	X1563	X1665	M1733	G1796	A1856	F1916	X1990	
	X1260	X1268	X1325	X1404	X1495	X1564	X1666	S1734	I1797	T1857	X1917	X1991	
	X1261	X1269	X1326	X1405	X1496	X1565	X1667	A1735	L1798	P1858	K1918		
	X1262	X1270	X1327	X1406	X1497	X1566	X1668	M1736	P1799	V1859	L1919	X1995	
	X1263	X1271	X1328	X1407	X1498	X1567	X1669	G1677	A1800	G1860	Q1920	X1996	
	X1264	X1272	X1329	X1408	X1499	X1568	X1670	F1737	D1801	R1861	K1921		
	X1265	X1273	X1330	X1409	X1500	X1569	X1671	E1738	A1802	V1862		X2000	
	X1266	X1274	X1331	X1410	X1501	X1570	X1672	E1739	T1803	L1863	I1924	X2001	
	X1267	X1275	X1332	X1411	X1502	X1571	X1673	T1740	F1804	A1864	I1925	X2002	
	X1268	X1276	X1333	X1412	X1503	X1572	X1674	V1741	G1805	S1865	E1926	X2003	
	X1269	X1277	X1334	X1421	X1504	X1573	X1675	T1742	A1806	L1866	L1927	X2004	
	X1270	X1278	X1335	X1422	X1505	X1574	X1676	D1743	G1807	F1867	Q1928	X2005	
	X1271	X1279	X1336	X1423	X1506	X1575	X1677	G1744	H1807	Q1868	R1929	X2006	
	X1272	X1280	X1337	X1424	X1507	X1576	X1678	X1745	S1808	E1869	X1930	X2007	
	X1273	X1281	X1338	X1425	X1508	X1577	X1679	L1746	L1809	A1870	L1931	X2008	
	X1274	X1282	X1339	X1426	X1509	X1578	X1680					X2009	
	X1275	X1283	X1340	X1429	X1510	X1579	X1681						
	X1276	X1284	X1341	X1430	X1511	X1580	X1682						
	X1277	X1285	X1342	X1431	X1512	X1581	X1683						
	X1278	X1286	X1343	X1432	X1513	X1582	X1684						
	X1279	X1287	X1344	X1433	X1514	X1583	X1685						
	X1280	X1288	X1345	X1434	X1515	X1584	X1686						
	X1281	X1289	X1346	X1435	X1516	X1585	X1687						
	X1282	X1290	X1347	X1436	X1517	X1586	X1688						
	X1283	X1291	X1348	X1437	X1518	X1587	X1689						
	X1284	X1292	X1349	X1438	X1519	X1588	X1690						
	X1285	X1293	X1350	X1439	X1520	X1589	X1691						
	X1286	X1294	X1351	X1440	X1521	X1590	X1692						
	X1287	X1295	X1352	X1441	X1522	X1591	X1693						
	X1288	X1296	X1353	X1442	X1523	X1592	X1694						
	X1289	X1297	X1354	X1443	X1524	X1593	X1695						
	X1290	X1298	X1355	X1444	X1525	X1594	X1696						
	X1291	X1299	X1356	X1445	X1526	X1595	X1697						
	X1292	X1300	X1357	X1446	X1527	X1596	X1698						
	X1293	X1301	X1358	X1447	X1528	X1597	X1699						
	X1294	X1302	X1359	X1448	X1529	X1598	X1700						
	X1295	X1303	X1360	X1449	X1530	X1599	X1701						
	X1296	X1304	X1361	X1450	X1531	X1600	X1702						
	X1297	X1305	X1362	X1451	X1532	X1601	X1703						
	X1298	X1306	X1363	X1452	X1533	X1602	X1704						
	X1299	X1307	X1364	X1453	X1534	X1603	X1705						
	X1300	X1308	X1365	X1454	X1535	X1604	X1706						
	X1301	X1309	X1366	X1455	X1536	X1605	X1707						
	X1302	X1310	X1367	X1456	X1537	X1606	X1708						
	X1303	X1311	X1368	X1457	X1538	X1607	X1709						
	X1304	X1312	X1369	X1458	X1539	X1608	X1710						
	X1305	X1313	X1370	X1459	X1540	X1609	X1711						
	X1306	X1314	X1371	X1460	X1541	X1610	X1712						
	X1307	X1315	X1372	X1461	X1542	X1611	X1713						
	X1308	X1316	X1373	X1462	X1543	X1612	X1714						
	X1309	X1317	X1374	X1463	X1544	X1613	X1715						
	X1310	X1318	X1375	X1464	X1545	X1614	X1716						
	X1311	X1319	X1376	X1465	X1546	X1615	X1717						
	X1312	X1320	X1377	X1466	X1547	X1616	X1718						
	X1313	X1321	X1378	X1467	X1548	X1617	X1719						
	X1314	X1322	X1379	X1468	X1549	X1618	X1720						
	X1315	X1323	X1380	X1469	X1550	X1619	X1721						
	X1316	X1324	X1381	X1470	X1551	X1620	X1722						
	X1317	X1325	X1382	X1471	X1552	X1621	X1723						
	X1318	X1326	X1383	X1472	X1553	X1622	X1724						
	X1319	X1327	X1384	X1473	X1554	X1623	X1725						
	X1320	X1328	X1385	X1474	X1555	X1624	X1726						
	X1321	X1329	X1386	X1475	X1556	X1625	X1727						
	X1322	X1330	X1387	X1476	X1557	X1626	X1728						
	X1323	X1331	X1388	X1477	X1558	X1627	X1729						
	X1324	X1332	X1389	X1478	X1559	X1628	X1730						



● Molecule 3: Tail protein



● Molecule 3: Tail protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	231.34Å 231.34Å 754.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 4.00 59.69 – 3.91	Depositor EDS
% Data completeness (in resolution range)	98.7 (60.00-4.00) 97.4 (59.69-3.91)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.319 , 0.346 0.299 , 0.333	Depositor DCC
R_{free} test set	8857 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	152.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 180.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	71862	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.80	7/8414 (0.1%)	0.95	28/11377 (0.2%)
1	D	0.80	7/8414 (0.1%)	0.95	32/11377 (0.3%)
1	G	0.82	7/8414 (0.1%)	0.96	29/11377 (0.3%)
2	B	0.41	0/6495	0.72	2/8812 (0.0%)
2	E	0.40	0/6495	0.72	3/8812 (0.0%)
2	H	0.41	0/6495	0.72	2/8812 (0.0%)
All	All	0.66	21/44727 (0.0%)	0.86	96/60567 (0.2%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1150	ASP	CB-CG	33.05	2.21	1.51
1	D	1150	ASP	CB-CG	32.65	2.20	1.51
1	A	1150	ASP	CB-CG	32.54	2.20	1.51
1	D	1181	PHE	CD2-CE2	21.08	1.81	1.39
1	G	1181	PHE	CE2-CZ	20.68	1.76	1.37

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1150	ASP	CB-CG-OD1	12.15	129.24	118.30
1	D	1150	ASP	CB-CG-OD1	12.14	129.22	118.30
1	A	1150	ASP	CB-CG-OD1	11.62	128.76	118.30
1	D	992	PHE	C-N-CD	-11.23	95.89	120.60
1	G	992	PHE	C-N-CD	-10.81	96.82	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11319	0	8817	2535	24
1	D	11319	0	8818	2518	14
1	G	11319	0	8817	2527	24
2	B	12310	0	7819	1753	0
2	E	12310	0	7817	1770	0
2	H	12310	0	7816	1770	0
3	C	325	0	76	25	0
3	F	325	0	76	28	0
3	I	325	0	76	35	0
All	All	71862	0	50132	12923	38

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 106.

The worst 5 of 12923 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1181:PHE:CE2	1:G:1181:PHE:CZ	1.76	1.71
1:A:1181:PHE:CZ	1:A:1181:PHE:CE2	1.75	1.69
1:D:1181:PHE:CD2	1:D:1181:PHE:CE2	1.81	1.68
1:G:1181:PHE:CE1	1:G:1181:PHE:CZ	1.75	1.68
1:D:1181:PHE:CD1	1:D:1181:PHE:CE1	1.78	1.66

The worst 5 of 38 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1150:ASP:OD1	1:D:1181:PHE:CE2[7_555]	1.80	0.40
1:A:1150:ASP:OD1	1:G:1181:PHE:CE2[7_555]	1.85	0.35
1:A:1181:PHE:CE2	1:G:1150:ASP:OD1[7_555]	1.85	0.35
1:D:1150:ASP:CG	1:D:1181:PHE:CE2[7_555]	1.87	0.33
1:A:1150:ASP:CG	1:G:1181:PHE:CE2[7_555]	1.87	0.33

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1069/1688 (63%)	401 (38%)	298 (28%)	370 (35%)	0	0
1	D	1069/1688 (63%)	396 (37%)	307 (29%)	366 (34%)	0	0
1	G	1069/1688 (63%)	398 (37%)	307 (29%)	364 (34%)	0	0
2	B	817/2006 (41%)	356 (44%)	245 (30%)	216 (26%)	0	1
2	E	817/2006 (41%)	357 (44%)	244 (30%)	216 (26%)	0	1
2	H	817/2006 (41%)	352 (43%)	247 (30%)	218 (27%)	0	0
All	All	5658/11082 (51%)	2260 (40%)	1648 (29%)	1750 (31%)	0	0

5 of 1750 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ALA
1	A	723	ALA
1	A	724	LYS
1	A	741	SER
1	A	742	LYS

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	871/895 (97%)	700 (80%)	171 (20%)	1	8
1	D	871/895 (97%)	697 (80%)	174 (20%)	1	8
1	G	871/895 (97%)	696 (80%)	175 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	703/703 (100%)	623 (89%)	80 (11%)	5	25
2	E	703/703 (100%)	623 (89%)	80 (11%)	5	25
2	H	703/703 (100%)	622 (88%)	81 (12%)	5	25
All	All	4722/4794 (98%)	3961 (84%)	761 (16%)	2	15

5 of 761 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1297	PRO
2	E	28	PHE
2	H	199	ILE
1	D	1354	GLU
1	D	1538	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1351	ASN
2	E	221	ASN
2	H	331	ASN
1	D	1389	GLN
1	D	1570	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	2
1	A	2
1	D	2

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	506:UNK	C	516:UNK	N	28.27
1	A	506:UNK	C	516:UNK	N	28.26
1	G	506:UNK	C	516:UNK	N	28.26
1	D	305:UNK	C	360:UNK	N	17.84
1	A	305:UNK	C	360:UNK	N	17.83

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1069/1688 (63%)	-0.35	0 100 100	48, 122, 192, 203	0
1	D	1069/1688 (63%)	-0.32	2 (0%) 95 93	53, 123, 194, 203	0
1	G	1069/1688 (63%)	-0.37	1 (0%) 95 94	43, 112, 190, 203	0
2	B	818/2006 (40%)	-0.12	25 (3%) 49 38	107, 177, 202, 203	0
2	E	818/2006 (40%)	-0.10	14 (1%) 70 60	111, 190, 202, 203	0
2	H	818/2006 (40%)	-0.15	17 (2%) 63 54	94, 183, 202, 203	0
3	C	0/65	-	-	-	-
3	F	0/65	-	-	-	-
3	I	0/65	-	-	-	-
All	All	5661/11277 (50%)	-0.25	59 (1%) 82 74	43, 151, 201, 203	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1895	ASN	9.5
2	H	451	ASN	4.7
2	H	51	ASP	4.3
2	E	1928	GLN	4.2
2	E	425	SER	4.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.